Lecture notes on topological insulators

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I. TOPOLOGICAL SUPERCONDUCTOR WITH TIME-REVERSAL SYMMETRY

In this Chap, we discuss spinful p-wave SC with TRS. That is, the DIII class with $T^2=-1, P^2=1$

A. Symmetry of the Hamiltonian matrix

Under the type-I basis, the PH operator is $\mathsf{P}=\tau_x K\otimes 1$ (see previous Chap). We write a general 4×4 Hamiltonian matrix as,

$$\mathsf{H}_k=\begin{pmatrix} \mathsf{h}_k & \mathsf{g}_k \\ \mathsf{g}_k^\dagger & \mathsf{h}'_k \end{pmatrix}. \tag{1.1}$$

Then $\mathsf{P}\mathsf{H}_k\mathsf{P}^{-1}=-\mathsf{H}_{-k}$ gives

$$\begin{pmatrix} \mathsf{h}'^*_k & \mathsf{g}_k^\dagger \\ \mathsf{g}_k^* & \mathsf{h}_k^* \end{pmatrix}=\begin{pmatrix} -\mathsf{h}_{-k} & -\mathsf{g}_{-k} \\ -\mathsf{g}_{-k}^\dagger & -\mathsf{h}'_{-k} \end{pmatrix}. \tag{1.2}$$

Therefore,

$$\begin{aligned} \mathsf{h}'_k &= -\mathsf{h}^*_{-k}, & (1.3)\\ \mathsf{g}_k^T &= -\mathsf{g}_{-k}. & (1.4) \end{aligned}$$

For the Hamiltonian matrix in Eq. (??), $\mathsf{g}_k=\bar{\Delta}_k$, and Eq. (1.4) is merely a restatement of Eq. (??), $\bar{\Delta}^\dagger(\mathbf{k})=-\bar{\Delta}^*(-\mathbf{k})$. The Hamiltonian matrix with PHS is thus of the form,

$$\mathsf{H}_k=\begin{pmatrix} \mathsf{h}_k & \mathsf{g}_k \\ \mathsf{g}_k^\dagger & -\mathsf{h}^*_{-k} \end{pmatrix}. \tag{1.5}$$

On the other hand, the TR operator for p-wave SC is $\mathsf{T}=1\otimes i\sigma_y K$. Then $\mathsf{T}\mathsf{H}_k\mathsf{T}^{-1}=\mathsf{H}_{-k}$ gives

$$\begin{pmatrix} \sigma_y\mathsf{h}_k^*\sigma_y & \sigma_y\mathsf{g}_k^*\sigma_y \\ \sigma_y\mathsf{g}_k^T\sigma_y & \sigma_y\mathsf{h}'^*_k\sigma_y \end{pmatrix}=\begin{pmatrix} \mathsf{h}_{-k} & \mathsf{g}_{-k} \\ \mathsf{g}_{-k}^\dagger & \mathsf{h}'_{-k} \end{pmatrix}. \tag{1.6}$$

Therefore,

$$\begin{aligned} \sigma_y\mathsf{h}_k^*\sigma_y &= \mathsf{h}_{-k}, \quad \text{(same for } \mathsf{h}'\text{)} & (1.7)\\ \sigma_y\mathsf{g}_k^*\sigma_y &= \mathsf{g}_{-k}. & (1.8) \end{aligned}$$

B. Chiral symmetry

The product of the TR operator and the PH operator is called the **chiral symmetry operator** S,

$$\mathsf{S}=\mathsf{T}\mathsf{P}, \tag{1.9}$$

which is an unitary operator. Its square, S^2, can be ± 1, depending on the signs of T^2 and P^2. But we usually only take $\mathsf{S}^2=1$, after redefining the phase of S (for $\mathsf{S}^2=-1$), $\mathsf{S}=\pm i\mathsf{T}\mathsf{P}$. Note that similar phase shift would not change the sign of T^2, P^2.

If a system has both TRS and PHS, then

$$\mathsf{S}\mathsf{H}_k\mathsf{S}^{-1}=\mathsf{T}\mathsf{P}\mathsf{H}_k\mathsf{P}^{-1}\mathsf{T}^{-1}=-\mathsf{H}_k. \tag{1.10}$$

That is, S is an unitary operator that *anti-commutes* with the Hamiltonian. In general, any unitary operator that anti-commutes with the Hamiltonian qualifies as a chiral symmetry operator (and the system is said to have the chiral symmetry). Note that a system cannot have chiral symmetry if one of the TR/PH symmetries is broken. However, when neither of the TR/PH symmetries exists, a system can still have chiral symmetry.

If H_k has chiral symmetry, then its eigenvalues would come in pairs with opposite signs:

$$\begin{aligned} \mathsf{H}_k\Phi_{nk} &= E_{nk}\Phi_{nk}, & (1.11)\\ \to\quad \mathsf{H}_k(\mathsf{S}\Phi_{nk}) &= -E_{nk}(\mathsf{S}\Phi_{nk}). & (1.12) \end{aligned}$$

Under the basis that diagonalizes S, a Hamiltonian with chiral symmetry has the standard form,

$$\mathsf{H}_k=\begin{pmatrix} 0 & \mathsf{f}_k \\ \mathsf{f}_k^\dagger & 0 \end{pmatrix}. \tag{1.13}$$

Note: The tight-binding Hamiltonian of a bipartite lattice with only nearest-neighbor couplings (sublattice-A couples with sublattice-B) can always be put in this form (if the on-site energies are all the same). Because we can assign the upper half of the basis to sublattice-A, and the lower half to sublattice-B. Then, there must exist an unitary matrix S that anti-commutes with H. That is, such a bipartite lattice has the chiral symmetry.

Suppose the eigenstates of H are $(\boldsymbol{\psi}_n,\boldsymbol{\phi}_n)^T, n=1,\cdots,N$, then

$$\begin{pmatrix} 0 & \mathsf{f} \\ \mathsf{f}^\dagger & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{\psi}_n^\pm \\ \boldsymbol{\phi}_n^\pm \end{pmatrix}=\pm\varepsilon_n\begin{pmatrix} \boldsymbol{\psi}_n^\pm \\ \boldsymbol{\phi}_n^\pm \end{pmatrix}, \varepsilon_n\ge 0. \tag{1.14}$$

It follows that (for either sign)

$$\begin{aligned} \mathsf{f}\,\mathsf{f}^\dagger\boldsymbol{\psi}_n &= \varepsilon_n^2\boldsymbol{\psi}_n, & (1.15)\\ \mathsf{f}^\dagger\mathsf{f}\,\boldsymbol{\phi}_n &= \varepsilon_n^2\boldsymbol{\phi}_n. & (1.16) \end{aligned}$$

Both $\boldsymbol{\psi}_n$ and $\boldsymbol{\phi}_n$ are assumed to be normalized, $\boldsymbol{\psi}_n^\dagger\boldsymbol{\psi}_n=\boldsymbol{\phi}_n^\dagger\boldsymbol{\phi}_n=1$. Then the normalized eigenstates are (for

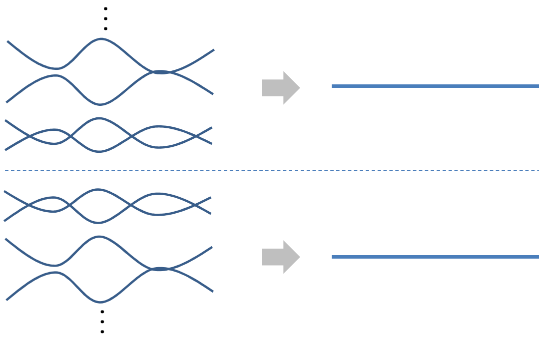

FIG. 1 The energy gap between filled states and empty states remains open during the spectral flattening.

$\varepsilon_n \neq 0$),

$$|\Psi_n^\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\psi_n^\pm \\ \phi_n^\pm\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}\psi_n \\ \pm\frac{\mathsf{f}^\dagger}{\varepsilon_n}\psi_n\end{pmatrix}. \tag{1.17}$$

As an example, consider the 4×4 Hamiltonian in Eq. (1.1) with both TRS and PHS,

$$\begin{aligned}\mathsf{S} \equiv -i\mathsf{TP} &= \begin{pmatrix}0 & \sigma_y \\ \sigma_y & 0\end{pmatrix} && (1.18)\\ &= \mathsf{U}\begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}\mathsf{U}^{-1}, && (1.19)\end{aligned}$$

where

$$\mathsf{U} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & \sigma_y \\ \sigma_y & -1\end{pmatrix}. \tag{1.20}$$

With the help of Eq. (1.10), one can show that,

$$\mathsf{U}\mathsf{H}_k\mathsf{U}^{-1} = \begin{pmatrix}0 & \mathsf{h}_k\sigma_y - \mathsf{g}_k \\ \sigma_y\mathsf{h}_k - \mathsf{g}_k^\dagger & 0\end{pmatrix}. \tag{1.21}$$

That is,

$$\mathsf{f}_k = \mathsf{h}_k\sigma_y - \mathsf{g}_k. \tag{1.22}$$

Also, the PH operator and the TR operator become,

$$\begin{aligned}\mathsf{U}\mathsf{P}\mathsf{U}^{-1} &= \begin{pmatrix}0 & -K \\ -K & 0\end{pmatrix} = -\sigma_x K \otimes 1, && (1.23)\\ \mathsf{U}\mathsf{T}\mathsf{U}^{-1} &= \begin{pmatrix}0 & -iK \\ iK & 0\end{pmatrix} = \sigma_y K \otimes 1. && (1.24)\end{aligned}$$

Eqs. (1.3) and (1.4) remain valid, while Eqs. (1.7) and (1.8) become

$$\begin{aligned}\mathsf{h}_k^* &= \mathsf{h}_{-k}, && (1.25)\\ \mathsf{g}_k^T &= -\mathsf{g}_{-k}. && (1.26)\end{aligned}$$

C. Topology of system with chiral symmetry

We first discuss systems with only chiral symmetry (class AIII). Other symmetry would impose further constraint on the Hamiltonian matrix and is discussed later.

1. Spectral flattening

If we are only interested in topological properties, then the trick of **spectral flattening** can be employed (see Fig. 1),

$$\pm\,\varepsilon_{nk} \to \pm 1. \tag{1.27}$$

The *flattened* Hamiltonian can be written in projection operators, which are defined as,

$$\begin{aligned}\mathsf{P}_k^\pm &= \sum_{n=1}^N |\Psi_n^\pm\rangle\langle\Psi_n^\pm| && (1.28)\\ &= \frac{1}{2}\sum_{n=1}^N \begin{pmatrix}\psi_n^\pm \\ \phi_n^\pm\end{pmatrix}\left(\psi_n^{\pm\dagger}, \phi_n^{\pm\dagger}\right). && (1.29)\end{aligned}$$

Then, the flattened Hamiltonian $\mathsf{H}_k \to \mathsf{Q}_k$ is,

$$\begin{aligned}\mathsf{Q}_k &= \sum_{n=1}^N \left(|\Psi_n^+\rangle\langle\Psi_n^+| - |\Psi_n^-\rangle\langle\Psi_n^-|\right) && (1.30)\\ &= 1 - 2\mathsf{P}_k^- && (1.31)\\ &= \sum_{n=1}^N \begin{pmatrix}0 & \psi_n\psi_n^\dagger\frac{\mathsf{f}}{\varepsilon_n} \\ \frac{\mathsf{f}^\dagger}{\varepsilon_n}\psi_n\psi_n^\dagger & 0\end{pmatrix} && (1.32)\\ &= \begin{pmatrix}0 & \mathsf{q}_k \\ \mathsf{q}_k^\dagger & 0\end{pmatrix}, && (1.33)\end{aligned}$$

with

$$\mathsf{q}_k = \sum_{n=1}^N \psi_{nk}\psi_{nk}^\dagger\frac{\mathsf{f}_k}{\varepsilon_{nk}}. \tag{1.34}$$

The eigenstates of Q_k with eigenvalues ± 1 now become,

$$|\Phi_{nk}^\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\eta_n \\ \pm\mathsf{q}_k^\dagger\eta_n\end{pmatrix}, \text{ where } (\eta_n)_a = \delta_{na};\ a = 1,\cdots,N. \tag{1.35}$$

2. Singular value decomposition

Using the **singular-value decomposition** (SVD), which applies to *any* complex matrix, the off-diagonal blocks can be decomposed as,

$$\mathsf{f}_k = \mathsf{u}_k^\dagger\mathsf{d}_k\mathsf{v}_k, \tag{1.36}$$

where d_k is diagonal with (non-negative) real elements, and u_k, v_k are unitary. It follows that,

$$\begin{aligned}\mathsf{H}_k &= \begin{pmatrix}0 & \mathsf{u}_k^\dagger\mathsf{d}_k\mathsf{v}_k \\ \mathsf{v}_k^\dagger\mathsf{d}_k\mathsf{u}_k & 0\end{pmatrix} && (1.37)\\ &= \frac{1}{\sqrt{2}}\begin{pmatrix}\mathsf{u}_k^\dagger & \mathsf{u}_k^\dagger \\ \mathsf{v}_k^\dagger & -\mathsf{v}_k^\dagger\end{pmatrix}\begin{pmatrix}\mathsf{d}_k & 0 \\ 0 & -\mathsf{d}_k\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}\mathsf{u}_k & \mathsf{v}_k \\ \mathsf{u}_k & -\mathsf{v}_k\end{pmatrix}.\end{aligned}$$

The $2N\times 2N$ diagonal matrix is flanked by unitary matrices. Therefore, the eigenvalues of H_k are the eigenvalues of d_k (positive) and $-\mathsf{d}_k$ (negative). After spectral flattening, $\pm\mathsf{d}_k\rightarrow\pm 1$, and

$$\mathsf{q}_k=\mathsf{u}_k^\dagger\mathsf{v}_k\ \in U(N). \tag{1.38}$$

The topology of the chiral system is given by the winding number of the mapping $\mathbf{k}(\in BZ)\rightarrow\mathsf{q}_k$.

3. Topology

If the BZ (a torus) can be replaced by a sphere S^D, that is, the effect of lattice can be ignored, then we can rely on the homotopy theory to get these winding numbers. For example, it is known that (Actor, 1979),

$$\begin{aligned}\pi_1(U(N)) &= Z \text{ for } N\geq 1 && (1.39)\\ \pi_2(U(N)) &= 0 \text{ for } N\geq 1 && (1.40)\\ (\text{In fact, } \pi_2(G) &= 0 \text{ for any Lie group } G)\\ \pi_3(U(1))=0, \pi_3(U(N)) &= Z \text{ for } N\geq 2. && (1.41)\end{aligned}$$

In general, for a large enough N, the result is "stabilized",

$$\pi_{2d}(\mathsf{U})=0,\ \pi_{2d+1}(\mathsf{U})=Z. \tag{1.42}$$

Therefore, we expect a chiral system in even dimension to be topologically trivial. In odd dimension, the topology is characterized by the winding number,

$$\begin{aligned}\nu_{2n+1} &= N_d\int_{BZ}d^{2d+1}k\ \epsilon_{ab\cdots}\mathrm{tr}\left(\mathsf{q}^\dagger\partial_a\mathsf{q}\mathsf{q}^\dagger\partial_b\mathsf{q}\cdots\right) && (1.43)\\ &= N_d\int_{BZ}\mathrm{tr}\left(\mathsf{q}^\dagger d\mathsf{q}\right)^{2d+1}, && (1.44)\\ N_d &= -\frac{d!}{(2d+1)!(2\pi i)^{d+1}}, && (1.45)\end{aligned}$$

and the second equation is written in differential form.

For example,

$$\begin{aligned}\nu_1 &= \frac{i}{2\pi}\int_{BZ}dk\mathrm{tr}\left(\mathsf{q}^\dagger\partial_k\mathsf{q}\right) && (1.46)\\ &= \frac{1}{2\pi i}\int_{BZ}dk\partial_k\ln\det\mathsf{q}_k, && (1.47)\end{aligned}$$

and

$$\nu_3=\frac{1}{24\pi^2}\int_{BZ}d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{q}^\dagger\partial_a\mathsf{q}\mathsf{q}^\dagger\partial_b\mathsf{q}\mathsf{q}^\dagger\partial_c\mathsf{q}\right). \tag{1.48}$$

For more details, see the Supp material of Schnyder and Ryu, 2011. Condensed matter systems with chiral symmetry (only) are rare in real world.

4. Constraint from other symmetry

If in addition to the chiral symmetry, the system has PHS and TRS, $\mathsf{P}^2=1,\mathsf{T}^2=-1$ (class DIII), then from either of the symmetries, we get $\mathsf{f}_k^T=-\mathsf{f}_{-k}$, or $\mathsf{q}_k^T=-\mathsf{q}_{-k}$. As a result, the winding number could be zero, instead of Z, in some odd dimensions. This is proved as follows (Ryu *et al.*, 2010):

$$\begin{aligned}&\mathrm{tr}\left[\mathsf{q}^\dagger(\mathbf{k})\frac{\partial\mathsf{q}(\mathbf{k})}{\partial k_a}\ \mathsf{q}^\dagger(\mathbf{k})\frac{\partial}{\partial k_b}\mathsf{q}(\mathbf{k})\cdots\right] && (1.49)\\ =\ &\mathrm{tr}\left[\mathsf{q}^*(-\mathbf{k})\frac{\partial\mathsf{q}^T(-\mathbf{k})}{\partial k_a}\ \mathsf{q}^*(-\mathbf{k})\frac{\partial}{\partial k_b}\mathsf{q}^T(-\mathbf{k})\cdots\right] && (1.50)\\ =\ &\mathrm{tr}\left[\mathsf{q}^\dagger(-\mathbf{k})\frac{\partial\mathsf{q}(-\mathbf{k})}{\partial(-k_a)}\ \mathsf{q}^\dagger(-\mathbf{k})\frac{\partial}{\partial(-k_b)}\mathsf{q}(-\mathbf{k})\cdots\right]^*, && (1.51)\end{aligned}$$

where we have used $\mathsf{q}^\dagger\partial_a\mathsf{q}=-(\partial_a\mathsf{q}^\dagger)\mathsf{q}$ in the last equation. It follows that,

$$\nu_{2d+1}=(-1)^{d+1}\nu_{2d+1}^*, \tag{1.52}$$

in which $(-1)^{d+1}$ comes from the imaginary number i in N_d. As a result, $\nu_{2d+1}=0$ when $2d+1=1,5,9\cdots$.

Even though the winding number for class-DIII materials in dimension $D=1,2$ is zero, other topological characterization is possible. At a TRIM Λ, q_Λ is anti-symmetric, $\mathsf{q}_\Lambda^T=-\mathsf{q}_\Lambda$ (see Eq. 1.26). This reminds us of the sewing matrix of a topological insulator in Chap **??**. In fact, for a p-wave SC with TRS ($\mathsf{T}^2=-1$), one can cook up a similar Z_2 topological number (for $D=1,2$), as shown below. For $D=3$, the topological number is the one in Eq. (1.48).

Following Schnyder and Ryu, 2011, define the sewing matrix,

$$w_{mn}(\mathbf{k})=\langle\Phi_m^+(-\mathbf{k})|\mathsf{T}\Phi_n^+(\mathbf{k})\rangle, \tag{1.53}$$

in which

$$\mathsf{T}=\sigma_y K\otimes 1. \tag{1.54}$$

As a result,

$$\begin{aligned}w_{mn}(\mathbf{k}) &= \frac{1}{2}(\boldsymbol{\eta}_m^\dagger,\boldsymbol{\eta}_m^\dagger\mathsf{q}_{-k})(\sigma_y K\otimes 1)\begin{pmatrix}\boldsymbol{\eta}_n\\ \mathsf{q}_k^\dagger\boldsymbol{\eta}_n\end{pmatrix} && (1.55)\\ &= q_{mn}^T(\mathbf{k})/i. && (1.56)\end{aligned}$$

Note that $m,n=1,\cdots N$, in which N is an even integer because of the two spin degrees of freedom.

Analogous to the topological insulator, one can define a Kane-Mele topological number (see **??**),

$$\begin{aligned}(-1)^\nu &= \prod_a\frac{\mathrm{Pf}\ [\mathsf{w}(\Lambda_a)]}{\sqrt{\det[\mathsf{w}(\Lambda_a)]}} && (1.57)\\ &= \prod_a\frac{\mathrm{Pf}\ [\mathsf{q}^T(\Lambda_a)/i]}{\sqrt{\det[\mathsf{q}^T(\Lambda_a)/i]}}=\pm 1. && (1.58)\end{aligned}$$

D. 1D and 2D system

Recall that the QWZ model of QAHE has chiral edge state and breaks TRS. The BHZ model for QSHE, which

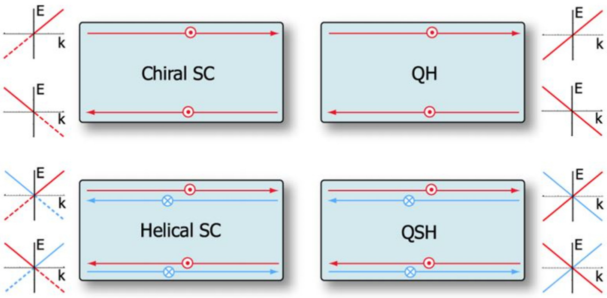

FIG. 2 Chiral superconductor, helical superconductor, and their edge states. Quantum Hall system and quantum spin Hall system are also plotted for comparison. The figure is from Qi *et al.*, 2009.

consists of a QWZ model and its time-reversal partner, has helical edge state and TRS. Here, similarly, the spinless p-wave superconductors in previous chapters have chiral edge state and no TRS. One can construct a SC with TRS using a time-reversal conjugate pair of p-wave superconductors (Fig. 2).

1. 1D and 2D model

In the Kitaev model of 1D p-wave SC, we have the Hamiltonian (see Eq. (??)),

$$\mathsf{h}(\mathbf{k}) = \begin{pmatrix} -t\cos k - \mu & i\Delta_0 \sin k \\ -i\Delta_0 \sin k & t\cos k + \mu \end{pmatrix}, \tag{1.59}$$

with the basis $(c_k, c^\dagger_{-k})^T$. According to the recipe mentioned above, one can extend the basis to $(c_{k\uparrow}, c^\dagger_{-k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\downarrow})^T$, and build a TRS SC with the Hamiltonian,

$$\begin{aligned} \mathsf{H}_0 &= \begin{pmatrix} \varepsilon_k & i\Delta_0 \sin k & 0 & 0 \\ -i\Delta_0 \sin k & -\varepsilon_k & 0 & 0 \\ 0 & 0 & \varepsilon_k & i\Delta_0 \sin k \\ 0 & 0 & -i\Delta_0 \sin k & -\varepsilon_k \end{pmatrix} \\ &= \varepsilon_k \; 1 \otimes \tau_z - \Delta_0 \sin k \; 1 \otimes \tau_y, \end{aligned} \tag{1.60}$$

where $\varepsilon_k = -t\cos k - \mu$.

If the basis $(c_{k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\uparrow}, c^\dagger_{-k\downarrow})^T$ is used, then one first switches the 2nd and the 3rd rows, then switches the 2nd and the 3rd columns of the Hamiltonian matrix (i.e. switch the order of $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$). Furthermore, one can add a spin-orbit (SO) coupling with strength α (Liu *et al.*, 2014), such that

$$\begin{aligned} \mathsf{H} &= \varepsilon_k \tau_z \otimes 1 - \Delta_0 \sin k \; \tau_y \otimes 1 + \alpha \sin k \; \tau_z \otimes \sigma_y \\ &= \begin{pmatrix} \varepsilon_k & i\alpha \sin k & i\Delta_0 \sin k & 0 \\ -i\alpha \sin k & \varepsilon_k & 0 & i\Delta_0 \sin k \\ -i\Delta_0 \sin k & 0 & -\varepsilon_k & -i\alpha \sin k \\ 0 & -i\Delta_0 \sin k & i\alpha \sin k & -\varepsilon_k \end{pmatrix}, \end{aligned} \tag{1.61}$$

It can be verified that such a Hamiltonian does have both PHS and TRS.

The 1D model above can be generalized to 2D, as follows (Liu *et al.*, 2014),

$$\begin{aligned} \mathsf{H} &= \varepsilon_k \tau_z + \alpha \sin k_x \; \tau_z \otimes \sigma_y - \alpha \sin k_y \; \sigma_x \\ &- \Delta_0 \sin k_x \; \tau_y + \Delta_0 \sin k_y \; \tau_x \otimes \sigma_z, \end{aligned} \tag{1.62}$$

where $\varepsilon_k = -t(\cos k_x + \cos k_y) - \mu$. This corresponds to $\mathbf{d} = \Delta_0(-\sin k_y, \sin k_x, 0)$. Also, it can be shown that such a Hamiltonian does have both PHS and TRS. It reduces to the 1D model by setting $k_y = 0$.

Some remarks: Note that the normal-state Hamiltonian is of the form,

$$\mathsf{h}_k = \varepsilon_k + \boldsymbol{\ell}_{so}(\mathbf{k}) \cdot \boldsymbol{\sigma}, \tag{1.63}$$

where $\boldsymbol{\ell}_{so}(\mathbf{k}) = \alpha(-\sin k_y, \sin k_x, 0)$. It is chosen to be parallel to $\mathbf{d}(\mathbf{k})$, so that the SO coupling would not break electron pairs (Schnyder and Ryu, 2011).

Also, we ignore possible s-wave pairing that could be induced by the SO coupling (more details in Sec I.E). Thus, the SC model here has only p-wave pairing.

Noncentrosymmetric superconductors, such as the heavy-fermion material $CePt_3Si$, has intrinsic SO coupling. In reality, the energy scale of the SO coupling could be larger than the SC gap. See Yip, 2014 for more details.

2. Topological number

One can identify the blocks h_k and g_k defined in Eq. (1.1) as,

$$\mathsf{h}_k = \varepsilon_k + \alpha \sin k_x \; \sigma_y - \alpha \sin k_y \; \sigma_x, \tag{1.64}$$

$$\mathsf{g}_k = i\Delta_0 \sin k_x + \Delta_0 \sin k_y \; \sigma_z. \tag{1.65}$$

It can be verified that Eqs. (1.3),(1.4),(1.7), and (1.8) are all satisfied. Also,

$$\begin{aligned} \mathsf{f}_k &= \mathsf{h}_k \sigma_y - \mathsf{g}_k \\ &= \varepsilon_k \sigma_y + (\alpha - i\Delta_0) \sin k_x - i(\alpha - i\Delta_0) \sin k_y \; \sigma_z. \end{aligned} \tag{1.66}$$

It follows that,

$$\begin{aligned} \mathsf{f}_k \mathsf{f}_k^\dagger &= \varepsilon_k^2 + (\alpha^2 + \Delta_0^2)\left(\sin^2 k_x + \sin^2 k_y\right) \\ &- 2\alpha\varepsilon_k \begin{pmatrix} 0 & \sin k_y + i \sin k_x \\ \sin k_y - i \sin k_x & 0 \end{pmatrix}, \end{aligned} \tag{1.67}$$

which has the eigenvalues,

$$\begin{aligned} \lambda_\pm (= \varepsilon_{k\pm}^2) &= \varepsilon_k^2 + (\alpha^2 + \Delta_0^2)\left(\sin^2 k_x + \sin^2 k_y\right) \\ &\pm \; 2\alpha\varepsilon_k \sqrt{\sin^2 k_x + \sin^2 k_y}. \end{aligned} \tag{1.68}$$

The corresponding eigenvectors are,

$$\psi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \frac{-\sin k_y + i \sin k_x}{\sqrt{\sin^2 k_x + \sin^2 k_y}} \end{pmatrix}. \tag{1.69}$$

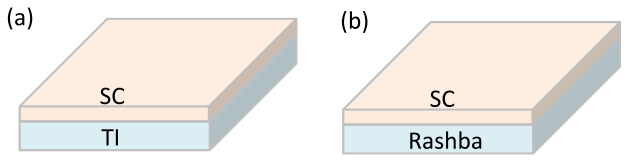

FIG. 3 Hybrid structure of (a) superconductor and topological insulator, (b) superconductor and semiconductor QW with Rashba SO coupling.

Note that at TRIM, there are removable singularities and the eigenvectors remain finite. From these, we can get the flattened off-diagonal part q_Λ, and determine the Z_2 topological number ν.

It is left as an exercise (Ex. 3) to show that in 1D, $|\mu| < t$ is a topological phase with $\nu = 1$, while $|\mu| > t$ is a trivial phase with $\nu = 0$ (Liu *et al.*, 2014). The 2D case can also be determined in the same way.

E. Hybrid structure

P-wave superconductors are rare in nature. However, it is possible to have effective p-wave pairing using hybrid structures that combine SC with SO coupling (see Fig. 3). This comes with two types: SC/TI, and SC/Rashba (both in 2D). They can be described within the same framework (e.g., see Santos *et al.*, 2010).

In the hybrid structure, a SC layer is attached to a TI. Because of the **proximity effect** (that is, Cooper pairs would leak to the TI), the 2D surface-state electrons of TI would feel both the SO coupling (see Lect **??**) and the superconductivity. Because of the SO coupling, s-wave pairing could be transformed to p-wave pairing (see below), thus indigenous p-wave SC could be spared in experiments (Fu and Kane, 2008).

The TI can be replaced by semiconductor quantum well with Rashba (or other types of) SO coupling (Alicea, 2010; Sau *et al.*, 2010), and the 2D electron gas in the well would feel the superconductivity. One difference between this setup with the one above is that, for the Rashba system, the chemical potential would inevitably cut out two Fermi surfaces (see Fig. 4).

Let's begin with the type-II basis, $\bar{\Psi}_k = (c_{k\uparrow}, c_{k\downarrow}, c^\dagger_{-k\downarrow}, -c^\dagger_{-k\uparrow})^T$. The Hamiltonian matrix is

$$\mathsf{H}_k = \begin{pmatrix} \mathsf{h}_k & \Delta_k \\ \Delta_k^\dagger & -\sigma_y \mathsf{h}^T_{-k}\sigma_y \end{pmatrix}, \tag{1.70}$$

in which

$$\begin{aligned} \mathsf{h}_k &= \varepsilon_k^0 - \mu + \boldsymbol{\ell}_k\cdot\boldsymbol{\sigma}, & (1.71)\\ \Delta_k &= d_k^0 + \mathbf{d}_k\cdot\boldsymbol{\sigma}. & (1.72)\end{aligned}$$

For TI surface state, $\varepsilon_k^0 = 0$; for Rashba electron, $\varepsilon_k^0 = \hbar^2k^2/2m^*$. The z-component of $\boldsymbol{\ell}_k$ is zero if TRS is not broken, while the other two components depend on actual materials used.

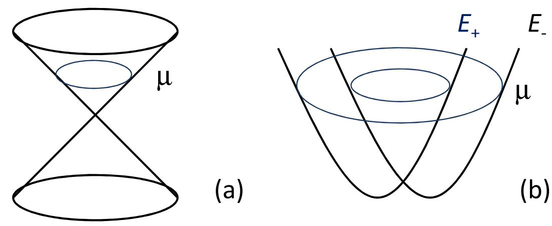

FIG. 4 The energy levels of (a) surface electron gas of topological insulator, (b) 2D electron gas with Rashba SO coupling.

The SO coupling breaks space-inversion symmetry, $\boldsymbol{\ell}_{-k} = -\boldsymbol{\ell}_k$. Thus it might mix superconducting pairs of even parity (s-wave) with odd parity (p-wave).

The eigenvalues and eigenvectors of h_k are,

$$\begin{aligned} \varepsilon_{k\pm} &= \varepsilon_k^0 - \mu \pm |\boldsymbol{\ell}_k|, & (1.73)\\ \boldsymbol{\psi}_{k\pm} &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm e^{i\varphi_k}\end{pmatrix}, & (1.74)\end{aligned}$$

where

$$e^{i\varphi_k} = \frac{\ell_{kx} + i\ell_{ky}}{\ell_k},\ \ \ell_k \equiv |\boldsymbol{\ell}_k| \neq 0. \tag{1.75}$$

Under time reversal, one has

$$\begin{aligned} \mathsf{T}\boldsymbol{\psi}_{k\uparrow} &= \boldsymbol{\psi}_{-k\downarrow}, & (1.76)\\ \mathsf{T}\boldsymbol{\psi}_{k\downarrow} &= -\boldsymbol{\psi}_{-k\uparrow}. & (1.77)\end{aligned}$$

Also, $e^{i\varphi_{-k}} = -e^{i\varphi_k}$ since $\boldsymbol{\ell}_k$ is odd in $\mathbf{k}$. Therefore,

$$\mathsf{T}\boldsymbol{\psi}_{k\pm} = \pm e^{-i\varphi_{-k}}\boldsymbol{\psi}_{-k\pm}. \tag{1.78}$$

Note that the TR operation does not flip the $\pm$-branch.

In terms of second quantization,

$$\begin{pmatrix} c_{k+} \\ c_{k-}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & +e^{-i\varphi_k} \\ 1 & -e^{-i\varphi_k}\end{pmatrix}\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}\end{pmatrix}, \tag{1.79}$$

or

$$\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ e^{i\varphi_k} & -e^{i\varphi_k}\end{pmatrix}\begin{pmatrix} c_{k+} \\ c_{k-}\end{pmatrix}, \tag{1.80}$$

then

$$\begin{pmatrix} c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ e^{i\varphi_k} & -e^{i\varphi_k}\end{pmatrix}\begin{pmatrix} -e^{-i\varphi_k}c^\dagger_{-k+} \\ e^{-i\varphi_k}c^\dagger_{-k-}\end{pmatrix}. \tag{1.81}$$

It is legitimate to assume that Cooper pairs are made of TR-conjugate electrons, so that

$$\Delta_{k\lambda} \sim \langle c_{-k\lambda}c_{k\lambda}\rangle,\ \ \lambda = \pm. \tag{1.82}$$

Define a new basis $\tilde{\Psi}_k = (c_{k+}, c_{k-}, e^{-i\varphi_k}c^\dagger_{-k+}, -e^{-i\varphi_k}c^\dagger_{-k-})^T$, which is related to the old one by an unitary transformation,

$$\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \\ c^\dagger_{-k\downarrow} \\ -c^\dagger_{-k\uparrow}\end{pmatrix} = \mathsf{U}\begin{pmatrix} c_{k+} \\ c_{k-} \\ e^{-i\varphi_k}c^\dagger_{-k+} \\ -e^{-i\varphi_k}c^\dagger_{-k-}\end{pmatrix}. \tag{1.83}$$

The Hamiltonian can be written in either basis,

$$H = \sum_{\mathbf{k}} \bar{\Psi}_k^\dagger \begin{pmatrix} \mathsf{h}_k & \Delta_k \\ \Delta_k^\dagger & -\sigma_y \mathsf{h}_{-k}^T \sigma_y \end{pmatrix} \bar{\Psi}_k \tag{1.84}$$

$$= \sum_{\mathbf{k}} \tilde{\Psi}_k^\dagger \begin{pmatrix} \tilde{\mathsf{h}}_k & \tilde{\Delta}_k \\ \tilde{\Delta}_k^\dagger & -\tilde{\mathsf{h}}_{-k}^T \end{pmatrix} \tilde{\Psi}_k, \tag{1.85}$$

where

$$\tilde{\mathsf{h}}_k = \begin{pmatrix} \varepsilon_{k+} & 0 \\ 0 & \varepsilon_{k-} \end{pmatrix} \tag{1.86}$$

$$\tilde{\Delta}_k = \begin{pmatrix} \Delta_{k+} & 0 \\ 0 & \Delta_{k-} \end{pmatrix}. \tag{1.87}$$

Both blocks are diagonal in the new basis, but not in the old basis.

After the unitary transformation $\mathsf{H} = \mathsf{U}\tilde{\mathsf{H}}\mathsf{U}^\dagger$, we have

$$\mathsf{h} = \begin{pmatrix} \varepsilon_k^0 - \mu & \ell_k e^{-i\varphi_k} \\ \ell_k e^{i\varphi_k} & \varepsilon_k^0 - \mu \end{pmatrix}, \tag{1.88}$$

$$\Delta_k = \begin{pmatrix} \Delta_{ks} & \Delta_{kt} e^{-i\varphi_k} \\ \Delta_{kt} e^{i\varphi_k} & \Delta_{ks} \end{pmatrix}, \tag{1.89}$$

$$= \underbrace{\Delta_{ks}}_{d_k^0} + \underbrace{\Delta_{kt}\hat{\boldsymbol{\ell}}_k}_{\mathbf{d}_k} \cdot \boldsymbol{\sigma} \tag{1.90}$$

in which,

$$\Delta_{ks} = \frac{1}{2}(\Delta_{k+} + \Delta_{k-}), \tag{1.91}$$

$$\Delta_{kt} = \frac{1}{2}(\Delta_{k+} - \Delta_{k-}). \tag{1.92}$$

Conversely,

$$\Delta_{k\pm} = \Delta_{ks} \pm \Delta_{kt} \tag{1.93}$$

$$= d_k^0 \pm \mathbf{d}_k \cdot \hat{\boldsymbol{\ell}}_k. \tag{1.94}$$

Note that $\mathbf{d}_k \parallel \boldsymbol{\ell}_k$. This is directly connected with the fact that the Cooper pairs are made of TR-conjugate electrons.

Furthermore, particle-hole symmetry requires (see Exercise 1)

$$\Delta_{-ks} = \Delta_{ks}, \ \Delta_{-kt} = \Delta_{kt} \tag{1.95}$$

$$\text{or } \Delta_{-k\lambda} = \Delta_{k\lambda}. \tag{1.96}$$

Time reversal symmetry requires

$$\Delta_{-ks} = \Delta_{ks}^*, \ \Delta_{-kt} = \Delta_{kt}^* \tag{1.97}$$

$$\text{or } \Delta_{-k\lambda} = \Delta_{k\lambda}^*. \tag{1.98}$$

Finally, the eigenvalues of the 4×4 Hamiltonian matrix are,

$$E_{k\lambda} = \pm\sqrt{\varepsilon_{k\lambda}^2 + \Delta_{k\lambda}^2}. \tag{1.99}$$

If one of Δ_{ks}, Δ_{kt} is zero, then $|\Delta_{k+}| = |\Delta_{k-}|$, and the excitation spectrum is two-fold degenerate; the degeneracy is lifted if both are non-zero.

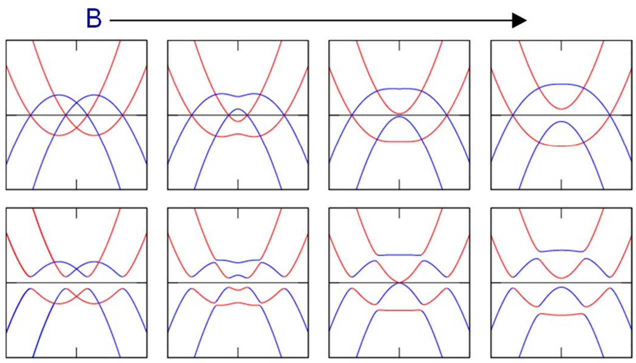

FIG. 5 The energy levels of SC/Rashba system under the influence of an magnetic field. The figures on the upper row are before turning on the SC gap, those on the the lower row are after. The figure is from Dr. Fleury's slide.

Under the new basis, the Hamiltonian in Eq. (1.85) is,

$$H = \sum_{k\lambda} \left[\varepsilon_{k\lambda} c_{k\lambda}^\dagger c_{k\lambda} + \lambda(e^{i\varphi_k}\Delta_{k\lambda} c_{-k\lambda} c_{k\lambda} + h.c.)\right]. \tag{1.100}$$

Let's reverse the logic and consider a special case: Assume a s-wave SC is used in the hybrid structure ($\boldsymbol{\ell}_k \neq 0$). That is, $\Delta_{ks} \neq 0, \Delta_{kt} = 0$, then $\Delta_{k+} = \Delta_{k-}$, and

$$H = \sum_{k\lambda} \left[\varepsilon_{k\lambda} c_{k\lambda}^\dagger c_{k\lambda} + \lambda(e^{i\varphi_k}\Delta_{ks} c_{-k\lambda} c_{k\lambda} + h.c.)\right]. \tag{1.101}$$

These two subsystems, $\lambda = \pm$, decouple with each other, and each one resembles the spinless p-wave SC in Eq. (**??**). Note that the angular dependence of the effective gap function, $e^{i\varphi_k}\Delta_{ks}$, is a result of the spin-momentum locking due to SO coupling (the factor $e^{i\varphi_k}$).

In the SC/TI structure, there is no fermion doubling, thus its effective Hamiltonian is just one of the subsystem. However, since the system has TRS, the edge state would not be chiral. TRS needs be broken to have non-degenerate Majorana fermions.

The same is true for the SC/Rashba structure. The degeneracy between two species of fermions needs be lifted by magnetic field or magnetic material to have stable Majorana fermions. See Fig. 5 for the effect of an external magnetic field on the energy levels.

For more information about experimental realization of such structures and detection of Majorana fermions, see Mourik *et al.*, 2012, Rokhinson *et al.*, 2012, Nadj-Perge *et al.*, 2014, Albrecht *et al.*, 2016, and Deng *et al.*, 2016.

Exercise:

1. For type-II basis, $\mathsf{P} = \tau_y \otimes \sigma_y K$. Show that PH symmetry gives the following constraint,

$$\mathsf{h}'_k = -\sigma_y \mathsf{h}_{-k}^* \sigma_y, \tag{1.102}$$

$$\mathsf{g}_k^T = \sigma_y \mathsf{g}_{-k} \sigma_y. \tag{1.103}$$

Since the TR operators are of the same form under two types of basis, so Eqs. (1.7) and (1.8) remain valid under type-II basis.

2. Suppose matrix S is unitary, with $\mathsf{S}^2 = 1$, and anti-commutes with H. Any basis state $\boldsymbol{\psi}_i$ $(i = 1, \cdots, 2N)$ can be decomposed as,

$$\begin{aligned} \boldsymbol{\psi}_i &= \frac{1}{2}(1+\mathsf{S})\boldsymbol{\psi}_i + \frac{1}{2}(1-\mathsf{S})\boldsymbol{\psi}_i \quad (1.104) \\ &\equiv \boldsymbol{\psi}_{i+} + \boldsymbol{\psi}_{i-}. \quad (1.105) \end{aligned}$$

Show that under the new basis,

$$\{\boldsymbol{\psi}_{1+}, \cdots, \boldsymbol{\psi}_{N+}; \boldsymbol{\psi}_{N+1,-}, \cdots, \boldsymbol{\psi}_{2N,-}\} \quad (1.106)$$

the two $N \times N$ off-diagonal blocks of S are zero, while the two $N \times N$ diagonal blocks of H are zero.

3. Given the 1D Hamiltonian in Eq. (1.61), evaluate its Kane-Mele topological number using Eq. (1.58). Show that (assume $t > 0$),

$$(-1)^\nu = \mathrm{sgn}(\mu + t)\mathrm{sgn}(\mu - t). \quad (1.107)$$

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